



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 03:58 am GMT

PDB ID : 3THF
Title : Crystal structure of the SD2 domain from Drosophila Shroom
Authors : Mohan, S.; VanDemark, A.P.
Deposited on : 2011-08-18
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

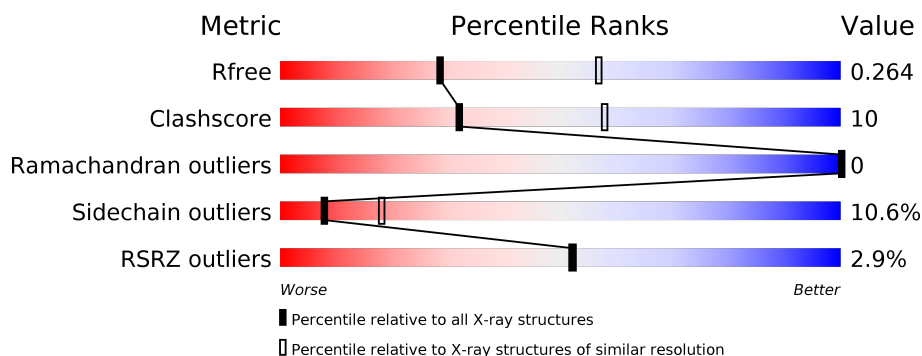
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	190	<div> <div>2%</div> <div> <div></div> <div>65%</div> <div>23%</div> <div>•</div> <div>8%</div> </div> </div>
1	B	190	<div> <div>3%</div> <div> <div></div> <div>66%</div> <div>22%</div> <div>•</div> <div>8%</div> </div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2749 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Protein Shroom.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	175	Total	C	N	O	S	0	0	0
			1378	846	249	277	6			
1	B	174	Total	C	N	O	S	0	0	0
			1371	842	248	275	6			

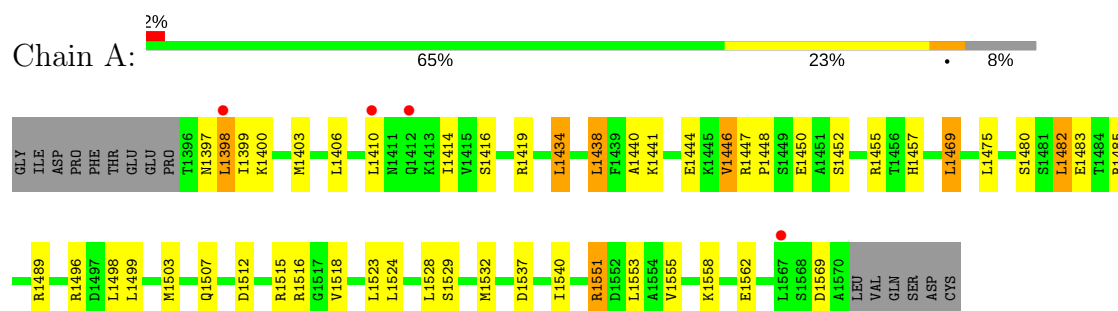
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1387	GLY	-	EXPRESSION TAG	UNP A1Z9P3
A	1388	ILE	-	EXPRESSION TAG	UNP A1Z9P3
A	1389	ASP	-	EXPRESSION TAG	UNP A1Z9P3
A	1390	PRO	-	EXPRESSION TAG	UNP A1Z9P3
A	1391	PHE	-	EXPRESSION TAG	UNP A1Z9P3
A	1392	THR	-	EXPRESSION TAG	UNP A1Z9P3
B	1387	GLY	-	EXPRESSION TAG	UNP A1Z9P3
B	1388	ILE	-	EXPRESSION TAG	UNP A1Z9P3
B	1389	ASP	-	EXPRESSION TAG	UNP A1Z9P3
B	1390	PRO	-	EXPRESSION TAG	UNP A1Z9P3
B	1391	PHE	-	EXPRESSION TAG	UNP A1Z9P3
B	1392	THR	-	EXPRESSION TAG	UNP A1Z9P3

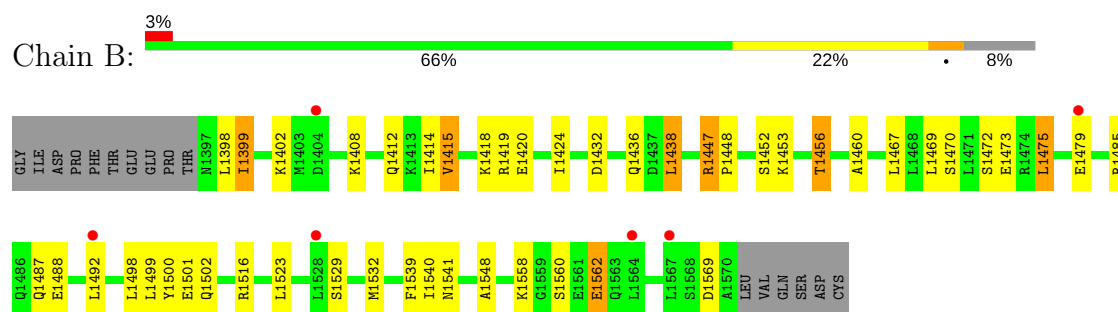
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Protein Shroom



• Molecule 1: Protein Shroom



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	72.80Å 85.63Å 92.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.63 – 2.70 47.63 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.9 (47.63-2.70) 98.8 (47.63-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.2_432)	Depositor
R, R_{free}	0.228 , 0.284 0.221 , 0.264	Depositor DCC
R_{free} test set	1177 reflections (7.19%)	DCC
Wilson B-factor (Å ²)	57.3	Xtriage
Anisotropy	0.753	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 63.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2749	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.28	0/1386	0.40	0/1854
1	B	0.29	0/1379	0.41	0/1844
All	All	0.29	0/2765	0.41	0/3698

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1378	0	1408	37	0
1	B	1371	0	1401	34	0
All	All	2749	0	2809	56	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (56) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1414:ILE:HD11	1:B:1560:SER:HB3	1.47	0.94
1:A:1496:ARG:HH11	1:A:1496:ARG:HG2	1.43	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1434:LEU:HD13	1:B:1539:PHE:HB2	1.68	0.76
1:A:1499:LEU:HB3	1:B:1475:LEU:HD22	1.70	0.73
1:A:1457:HIS:HA	1:B:1516:ARG:HH21	1.53	0.73
1:A:1553:LEU:HD12	1:B:1424:ILE:HD12	1.73	0.70
1:B:1412:GLN:O	1:B:1415:VAL:HG12	1.91	0.69
1:B:1414:ILE:O	1:B:1418:LYS:HG2	1.93	0.68
1:A:1457:HIS:HA	1:B:1516:ARG:NH2	2.09	0.67
1:A:1434:LEU:HD22	1:A:1438:LEU:HD22	1.77	0.66
1:B:1447:ARG:HG2	1:B:1448:PRO:HD2	1.78	0.66
1:B:1452:SER:O	1:B:1456:THR:HG22	1.97	0.65
1:B:1529:SER:H	1:B:1532:MET:HE3	1.64	0.62
1:A:1446:VAL:HG22	1:A:1450:GLU:OE1	2.01	0.61
1:A:1441:LYS:HG2	1:B:1532:MET:SD	2.40	0.61
1:A:1414:ILE:HD11	1:B:1560:SER:CB	2.27	0.57
1:A:1529:SER:OG	1:A:1532:MET:HG2	2.04	0.57
1:A:1480:SER:O	1:A:1483:GLU:HG2	2.05	0.56
1:B:1469:LEU:O	1:B:1473:GLU:HG3	2.06	0.56
1:A:1496:ARG:HG2	1:A:1496:ARG:NH1	2.18	0.55
1:B:1558:LYS:O	1:B:1562:GLU:HG2	2.07	0.55
1:B:1432:ASP:O	1:B:1436:GLN:HG3	2.08	0.53
1:A:1485:ARG:NH1	1:B:1488:GLU:HB3	2.26	0.51
1:B:1501:GLU:HG3	1:B:1502:GLN:N	2.26	0.50
1:B:1398:LEU:HG	1:B:1402:LYS:HE2	1.93	0.50
1:A:1496:ARG:HH11	1:A:1496:ARG:CG	2.19	0.48
1:A:1447:ARG:HG2	1:A:1448:PRO:HD2	1.95	0.48
1:A:1555:VAL:HA	1:A:1558:LYS:HD2	1.97	0.47
1:B:1453:LYS:HA	1:B:1456:THR:HG23	1.95	0.47
1:A:1469:LEU:HD21	1:B:1548:ALA:HA	1.95	0.47
1:A:1416:SER:O	1:A:1419:ARG:HB3	2.14	0.47
1:A:1503:MET:CE	1:A:1507:GLN:HE21	2.28	0.47
1:A:1524:LEU:HG	1:A:1528:LEU:HD12	1.96	0.47
1:B:1475:LEU:O	1:B:1479:GLU:HG2	2.15	0.47
1:A:1397:ASN:OD1	1:A:1400:LYS:HG2	2.15	0.46
1:A:1399:ILE:O	1:A:1403:MET:HG2	2.16	0.45
1:B:1398:LEU:O	1:B:1402:LYS:HG2	2.17	0.45
1:A:1496:ARG:CG	1:A:1496:ARG:NH1	2.79	0.45
1:B:1447:ARG:HG2	1:B:1448:PRO:CD	2.43	0.45
1:B:1438:LEU:HA	1:B:1438:LEU:HD12	1.82	0.44
1:A:1512:ASP:O	1:A:1515:ARG:HG2	2.17	0.44
1:A:1398:LEU:HA	1:A:1398:LEU:HD23	1.63	0.44
1:A:1469:LEU:HA	1:A:1469:LEU:HD12	1.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1498:LEU:O	1:B:1501:GLU:HG2	2.18	0.43
1:A:1537:ASP:O	1:A:1540:ILE:HG22	2.19	0.43
1:A:1440:ALA:O	1:A:1444:GLU:HG2	2.19	0.43
1:A:1551:ARG:HH22	1:B:1470:SER:HB2	1.84	0.43
1:A:1516:ARG:HH12	1:B:1460:ALA:HB3	1.84	0.43
1:B:1408:LYS:O	1:B:1412:GLN:HG3	2.19	0.42
1:A:1516:ARG:HH12	1:B:1460:ALA:CB	2.32	0.42
1:B:1540:ILE:HG23	1:B:1541:ASN:N	2.35	0.42
1:B:1399:ILE:HD12	1:B:1399:ILE:HA	1.83	0.42
1:A:1410:LEU:O	1:A:1414:ILE:HD13	2.19	0.41
1:A:1515:ARG:O	1:A:1518:VAL:HB	2.21	0.41
1:A:1553:LEU:HD11	1:B:1420:GLU:HG2	2.03	0.41
1:A:1482:LEU:HD13	1:B:1492:LEU:HD13	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	173/190 (91%)	172 (99%)	1 (1%)	0	100	100
1	B	172/190 (90%)	172 (100%)	0	0	100	100
All	All	345/380 (91%)	344 (100%)	1 (0%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	152/166 (92%)	136 (90%)	16 (10%)	8	18
1	B	151/166 (91%)	135 (89%)	16 (11%)	8	18
All	All	303/332 (91%)	271 (89%)	32 (11%)	8	18

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1398	LEU
1	A	1406	LEU
1	A	1434	LEU
1	A	1438	LEU
1	A	1446	VAL
1	A	1452	SER
1	A	1455	ARG
1	A	1469	LEU
1	A	1475	LEU
1	A	1482	LEU
1	A	1489	ARG
1	A	1498	LEU
1	A	1523	LEU
1	A	1551	ARG
1	A	1562	GLU
1	A	1569	ASP
1	B	1399	ILE
1	B	1415	VAL
1	B	1419	ARG
1	B	1438	LEU
1	B	1447	ARG
1	B	1456	THR
1	B	1467	LEU
1	B	1472	SER
1	B	1475	LEU
1	B	1485	ARG
1	B	1487	GLN
1	B	1499	LEU
1	B	1500	TYR
1	B	1523	LEU
1	B	1562	GLU
1	B	1569	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1507	GLN
1	B	1409	HIS
1	B	1507	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	175/190 (92%)	0.62	4 (2%) 61 61	41, 72, 105, 134	0
1	B	174/190 (91%)	0.65	6 (3%) 46 45	37, 72, 113, 146	0
All	All	349/380 (91%)	0.64	10 (2%) 52 52	37, 72, 110, 146	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1567	LEU	3.0
1	B	1528	LEU	2.7
1	A	1567	LEU	2.6
1	B	1404	ASP	2.6
1	A	1398	LEU	2.4
1	A	1410	LEU	2.2
1	B	1479	GLU	2.2
1	A	1412	GLN	2.1
1	B	1564	LEU	2.1
1	B	1492	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.